Comment on: Breakdown of Bohr's Correspondence Principle by: Bo Gao Phys. Rev. Lett. 83, 4225 (1999).

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Gao applied LeRoy and Bernstein [1] semi-classical analysis for the energy levels in a potential of the form $-C_n/r^n$ to sequences of scaled energy differences (SED) progressing towards low lying states and found a better agreement with the semi-classical prediction for low-lying levels until eventually interactions having shorter range come into play. The sequences given in his Table 1 are stopped before the agreement deteriorates. He claimed that Bohr's Correspondence Principle breaks down for all quantum systems in which the asymptotic interaction is of the form $1/r^n$ with $n > 2$.

We checked that for the energy levels obtained by Stwalley et al. [2] with the same potential [3], the agreement with the semi-classical approximation is better for higher vibrational quantum numbers in agreement with Bohr's correspondence principle.

Clearly a disagreement must exist between the energy levels calculated by Gao and those by Stwalley et al. for the same potential.

Thus we set out to evaluate directly the full spectrum of the Movre-Pichler [3] potential with a powerful tunable accuracy method that embodies a control of accuracy of the quantum eigenvalues. It is based on the Canonical Function Method (CFM) [4] that allows us to evaluate eigenvalues close to the ground state as well as close to highly excited states near the continuum. Hence the semi-classical approximation can be tested with high accuracy close to the continuum limit as well as at lower energies.

We used for the 0_g^- electronic state of the $^{23}Na_2$ molecule the same parameters as those of Stwalley et al. [2] who found 37 energy levels and extrapolated 3 extra ones. Our results along with Stwalley et al.'s (in cm^{-1}) and the corresponding SED are displayed in the Table progressing from the Ground up. The semi-classical approximation is better for higher vibrational quantum numbers as seen in the table (as compared to Gao's table 1) in our case and Stwalley et al.'s, except for our very last level (number 38) that is quite close to dissociation.

The fact that two entirely different and independent methods reached the same result leads us to believe that no breakdown of the Bohr's correspondence principle has been clearly established yet, in the above work.

Index	Stwalley et al.	SED	CFM	SED
1	-1.7887		-1.7864488	
2	-1.5617	0.9566	-1.5595638	0.9571
3	-1.3566	0.9698	-1.3546072	0.9702
4	-1.1723	0.9820	-1.1703990	0.9827
5	-1.0075	0.9939	-1.0057071	0.9946
6	-0.86087	1.0057	-0.8592631	1.0059
7	-0.73125	1.0159	-0.7297908	1.0164
8	-0.61729	1.0259	-0.6159534	1.0265
9	-0.51770	1.0352	-0.5164882	1.0358
10	-0.43120	1.0440	-0.4301217	1.0444
11	-0.35657	1.0520	-0.3556148	1.0525
12	-0.29261	1.0595	-0.2917693	1.0601
13	-0.23820	1.0662	-0.2374560	1.0669
14	-0.19224	1.0727	-0.1916002	1.0732
15	-0.15374	1.0783	-0.1531893	1.0789
16	-0.12176	1.0832	-0.1212854	1.0840
17	-9.5438(-02)	1.0873	-9.5022588(-02)	1.0886
18	-7.3940(-02)	1.0929	-7.3608452(-02)	1.0926
19	-5.6599(-02)	1.0957	-5.6325744(-02)	1.0962
20	-4.2754(-02)	1.0988	-4.2530867(-02)	1.0994
21	-3.1831(-02)	1.1014	-3.1650591(-02)	1.1021
22	-2.3323(-02)	1.1039	-2.3180420(-02)	1.1044
23	-1.6791(-02)	1.1058	-1.6679756(-02)	1.1064
24	-1.1854(-02)	1.1075	-1.1768655(-02)	1.1081
25	-8.1873(-03)	1.1088	-8.1228816(-03)	1.1094
26	-5.5165(-03)	1.1100	-5.4689541(-03)	1.1106
27	-3.6136(-03)	1.1109	-3.5793742(-03)	1.1115
28	-2.2916(-03)	1.1116	-2.2676168(-03)	1.1122
29	-1.3995(-03)	1.1122	-1.3831806(-03)	1.1128
30	-8.1747(-04)	1.1128	-8.0683859(-04)	1.1133
31	-4.5276(-04)	1.1132	-4.4613249(-04)	1.1138
32	-2.3503(-04)	1.1135	-2.3110168(-04)	1.1142

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[1] R.J. LeRoy and R.B. Bernstein, J. Chem. Phys. **52**, 3869 (1970).

[2] W.C. Stwalley, Y.H. Uang and G. Pichler, Phys. Rev. Lett. **41**, 1165 (1978).

[3] M. Movre and G. Pichler, J. phys. **B10**, 2631 (1977).

[4] C. Tannous, K. Fakhreddine and J. Langlois, J. Phys. IV France **9** Pr6-71 (1999).